Kondo effect in an antiferromagnetic metal

Vivek Aji,[1] Chandra M. Varma,[1] and Ilya Vekhter[2]

[1]*Department of Physics and Astronomy, University of California, Riverside, CA 92521*
[2]*Department of Physics and Astronomy, Louisiana State University, Baton Rouge LA 70803*

We study the fate of a spin-1/2 impurity in the itinerant antiferromagnetic metallic phase via a renormalization group analysis and a variational calculation. The local moment - conduction electron interaction hamiltonian in an antiferromagnetic metal is spin non-conserving. We show that for a general location of the impurity, the Kondo singularities still occur, but the ground state has a partially unscreened moment. We calculate the magnitude of this residual moment and the variation of the spin polarization with energy for a substitutional impurity as a function of the staggered magnetization. The usual Kondo effect only occurs if the impurity is placed at points where the magnetization is zero.

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I. INTRODUCTION.

The dual nature of electron behavior in antiferromagnetic (AFM) heavy fermion (HF) materials is not well understood. On one hand, in many intermetallic compounds containing elements with partially filled f-orbitals, the heavy mass originates from the collective screening of the local moments by the conduction band via the Kondo effect (for a review see Refs.1,2,3). Emergence of magnetic order, on the other hand, requires interaction between the unscreened moments.

In many materials exhibiting coexistence of antiferromagnetism and heavy mass the RKKY interaction between the local moments is comparable to the Kondo temperature[4,5], and the AFM order involves only *part* of the local moments at low temperatures[6]. This suggests a ground state where a fraction of the full unscreened moment appears as ordered staggered moment, while the rest continues to be compensated by the conduction electrons via the Kondo effect[6]. In materials with several f-electrons per unit cell, such as several U-containing compounds, the coexistence of AFM and HF behavior may be understood as originating from Kondo screening of one f-species and ordering of another. In systems with a single f-electron, for example many Ce-containing intermetallics, the coexistence of magnetic ordering and screening originates with the same local moment.

Motivated by this picture we consider in this paper the Kondo effect for a single impurity coupled to a band of conduction electrons that order antiferromagnetically. We believe that this is the first step towards developing a low-energy theory for the coexistence of the AFM and HF behavior. Just as the essential aspects of singlet formation and mass enhancement in paramagnetic heavy fermions follow from the analysis of the screening of a local moment in an electron bath, the salient features of competition between antiferromagnetism and Kondo screening can be understood from the analysis of our model. We write down a simple model hamiltonian for this problem and show that in a mean-field theory for the lattice, our model has precisely the local symmetries required to consider the competition between the two phenomena. We find that only partial screening of the impurity spin takes place due to spin non-conserving interaction vertices, with the unscreened moment fraction that depends on the amplitude of the AFM order.

A major advantage of our model is that it allows a variety of analytic approaches that make the underlying physical picture more transparent. Previous analyses of the competition between antiferromagnetism and screening for the Kondo lattice or equivalent models have been largely numerical. Several authors considered a half-filled Kondo lattice with anisotropic Kondo coupling[7,8]. In that case the AFM phase is insulating, rather than metallic, in contrast to the experimental situation. Moreover, the coexistence regime does not exist for the isotropic Kondo coupling that we consider, although it may appear under applied magnetic fields[9]. A metallic phase with coexisting Kondo screening and AFM order was recently found in variational Monte Carlo calculations for the Kondo Lattice Model[10], however, Kondo screening was argued to remain the same in the paramagnetic and antiferromagnetic phases, in contrast to our findings below.

Our study also has fundamental importance beyond the connection to the heavy fermion physics. Our main conclusions, (i) that the Kondo screening of an impurity placed in an itinerant antiferromagnet (a) depends on the location of the impurity within the unit cell; (b) for substitutional impurity on a simple lattice is incomplete with the magnitude of the residual moment related to the amplitude of the AFM order; (ii) that the spin-dependent local density of states reflects this incomplete screening can all be tested experimentally. It is important to emphasize that, for a system without nesting, after the onset of the AFM order and doubling of the unit cell there remains a large Fermi surface with non-vanishing density of states, and one may naively expect a complete Kondo screening. The existence of residual unscreened moment is due to the spin non-conserving vertices in the magnetically ordered state that alter the interaction between the conduction electron bath and the local moment.

The remainder of the paper is organized as follows. In the next section we introduce our model and discuss its

salient features. The structure of the interaction vertices and the renormalization group analysis are presented in Sec.III. We then present the variational ground state ansatz in Sec.IV, and follow it by the discussion of the density of states on the impurity site.

II. MODEL.

Our model consists of an electronic band with an itinerant AFM modulation coupled to an isolated impurity, with the hamiltonian $H = H_c + H_I + H_K$. The conduction band without magnetic order is described by

$$H_c = \sum_{\mathbf{k},\alpha} \varepsilon\left(\mathbf{k}\right) c^{\dagger}_{\mathbf{k},\alpha} c_{\mathbf{k},\alpha}\,, \tag{1}$$

where $\varepsilon\left(\mathbf{k}\right)$ is the energy band dispersion, and $c^{\dagger}_{\mathbf{k},\alpha}$ is the creation operator for an electron eigenstate in a paramagnet. The AFM order is imposed via

$$H_I = \sum_{\mathbf{k}} \left[\gamma m \left(c^{\dagger}_{\mathbf{k},\uparrow} c_{\mathbf{k}+\mathbf{Q},\uparrow} - c^{\dagger}_{\mathbf{k},\downarrow} c_{\mathbf{k}+\mathbf{Q},\downarrow}\right) + h.c.\right]\,, \tag{2}$$

where m is the mean field staggered magnetization, chosen along the spin z-axis, γm is the AFM gap, and $\mathbf{Q}$ is the ordering wave-vector.

We consider an isolated impurity with spin $\boldsymbol{S}$, at position $\mathbf{R}_i$ coupled antiferromagnetically to the fermion spins. The Kondo interaction is

$$H_K = -J \mathbf{S}_i \cdot \boldsymbol{\sigma}_{\alpha\beta} \psi^{\dagger}_{\alpha}(\mathbf{R}_i)\psi_{\beta}(\mathbf{R}_i)\,, \tag{3}$$

where J is the (Kondo) exchange coupling between the impurity spin and the conduction electrons, $\boldsymbol{\sigma}$ is the vector of Pauli matrices, and $\psi^{\dagger}_{\alpha}(\boldsymbol{R}) = \sum_{\mathbf{k}} c^{\dagger}_{\mathbf{k},\alpha} \exp(i\mathbf{k}\cdot\boldsymbol{R})$, is the creation operator in real space.

The justification for this model is as follows. Suppose we consider the full Kondo lattice Hamiltonian including the RKKY interaction and allow for the possibility of antiferromagnetic order so that the local spin at each site may be written as

$$\mathbf{S}_i = \langle \mathbf{S}_{\mathbf{Q}}\rangle \exp(i\mathbf{Q}\cdot\mathbf{R}_i) + \left[\mathbf{S}_i - \langle \mathbf{S}\rangle_{\mathbf{Q}} \exp(i\mathbf{Q}\cdot\mathbf{R}_i)\right]. \tag{4}$$

Now consider a mean field theory (for example the dynamical mean-field theory). At the first iteration of the self-consistent solution, one must solve the local "impurity" problem, without making this decomposition at the impurity site but making it everywhere else to generate a self-consistent bath. Then Eq.(2) follows as the periodic spin-dependent potential on the conduction electrons due to the staggered magnetization, $\gamma m \propto J\langle \boldsymbol{S}_{\boldsymbol{Q}}\rangle$. Therefore the local problem is precisely the problem with the symmetries of Eqs.(1)-(3). For a fully self-consistent solution we would have to relate γm to the sub-lattice moment generated at the impurity site(s) due to it; this second part is not attempted here. The self-consistency affects the quantitative details, but not qualitative physics of our conclusions. Our finding that there is only partial Kondo screening in the local model confirms the consistency of the approach.

In the absence of the Kondo coupling, the Hamiltonian, Eqs.(1)-(2) can be readily diagonalized using a Bogoliubov transformation. This introduces four species of fermions, described by the band indices $n = \pm$, in addition to the two spin projections on the z-axis $\alpha = \pm 1$.

$$\begin{pmatrix} a^{\dagger}_{+,\mathbf{k},\alpha} \\ a^{\dagger}_{-,\mathbf{k},\alpha} \end{pmatrix} = \begin{pmatrix} u_{\mathbf{k}} c^{\dagger}_{\mathbf{k},\alpha} - \alpha v_{\mathbf{k}} c^{\dagger}_{\mathbf{k}+\mathbf{Q},\alpha} \\ v_{\mathbf{k}} c^{\dagger}_{\mathbf{k},\alpha} + u_{\mathbf{k}} c^{\dagger}_{\mathbf{k}+\mathbf{Q},\alpha} \end{pmatrix}, \tag{5}$$

with the Bogoliubov factors

$$\left\{u^2_{\mathbf{k}}\,, v^2_{\mathbf{k}}\right\} = \frac{1}{2}\left[1 \pm \delta_{\mathbf{k}}/\sqrt{\delta^2_{\mathbf{k}} + \gamma^2 m^2}\right]. \tag{6}$$

Under this transformation the band hamiltonian becomes

$$H_b = H_c + H_I = \sum_{\mathbf{k},n,\alpha} E_n(\mathbf{k}) a^{\dagger}_{n\mathbf{k}\alpha} a_{n\mathbf{k}\alpha}\,, \tag{7}$$

with the energy dispersion $E_{\pm}(\mathbf{k}) = \xi_{\mathbf{k}} \pm \sqrt{\delta^2_{\mathbf{k}} + \gamma^2 m^2}$, and the shorthand notation $\xi_{\mathbf{k}} = \frac{1}{2}\left(\varepsilon(\mathbf{k}) + \varepsilon(\mathbf{k}+\mathbf{Q})\right)$ and $\delta_{\mathbf{k}} = \frac{1}{2}\left(\varepsilon(\mathbf{k}) - \varepsilon(\mathbf{k}+\mathbf{Q})\right)$. The momentum summation in Eq. (7) is over the first magnetic Brillouin Zone (MBZ). In the absence of nesting, $\xi_{\mathbf{k}} \neq 0$, the electrons remain ungapped, and the MBZ contains a Fermi surface (FS). Superficially, since the density of states at the Fermi level is finite, this may suggest that Kondo screening should occur as in a normal metal. We show below, however, that this is not the case since the Kondo interaction vertices have nontrivial spin structure.

The effective hamiltonian is now written in terms of the operators $a_{n,\mathbf{k},\alpha}$ as $H = H_b + H_K$ where H_b is given by Eq. (7), and the Kondo interaction is

$$H_K = -\frac{J}{2N} \sum_{\substack{\mathbf{k}\mathbf{k}' \\ nn'}} \mathbf{S}\cdot\boldsymbol{\sigma}_{\alpha\beta} f_{n\mathbf{k}\alpha} f^{\star}_{n'\mathbf{k}'\beta} a^{\dagger}_{n\mathbf{k}\alpha} a_{n'\mathbf{k}'\beta}\,, \tag{8a}$$

$$f_{+\boldsymbol{k}\alpha} = u_{\mathbf{k}} - \alpha v_{\mathbf{k}} e^{i\mathbf{Q}\mathbf{R}_i}\,, \tag{8b}$$

$$f_{-\boldsymbol{k}\alpha} = \alpha v_{\mathbf{k}} + u_{\mathbf{k}} e^{i\mathbf{Q}\mathbf{R}_i}\,. \tag{8c}$$

Again, the momentum summation in Eq. (8a) is over the first MBZ. Eq.(8a) shows that the effective Kondo interaction, written in terms of the eigenstates of the antiferromagnet is, in general, anisotropic, $\mathbf{k}$-dependent, as well as dependent on the location of the impurity in the lattice because of the structure factors, $f_{n\mathbf{k}\alpha}$. The impurity spin is coupled to fermions in both bands, and this interaction is weighted by the structure factors. Despite this apparent complication, we show below that the invariant vertices have a factorizable form so that the problem is still tractable.

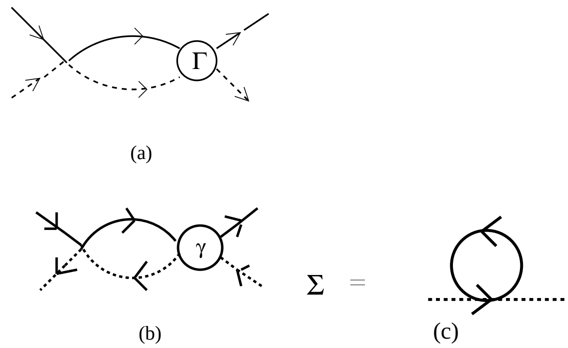

FIG. 1: a) Particle-Particle channel, (b) Particle-hole channel contributions to the vertex and (c) Contribution to the Pseudo-Fermion Self Energy

III. RENORMALIZATION GROUP ANALYSIS

A. Spin structure of invariant vertices

To identify the invariant vertices we employ the Abrikosov pseudo-fermion representation for the local moment, $\mathbf{S}=\sum_{\mu\nu}\boldsymbol{S}_{\mu\nu}\psi^\dagger_\mu\psi_\nu$, where $\boldsymbol{S}_{\mu\nu}$ is the spin matrix[11]. The integral equation for the interaction vertex is represented in Fig. 1 and contains contributions from the particle-particle (Fig. 1(a)) and the particle-hole (Fig. 1(b)) channels. For Fig. 1(a) we have ($k_B=\hbar=1$)

$$\begin{aligned}\Gamma^{\alpha\beta n}_{\alpha'\beta'n'}(\mathbf{k},\mathbf{k}') &= \frac{J}{2N}\left(\mathbf{S}_{\beta\beta'}\cdot\boldsymbol{\sigma}_{\alpha\alpha'}\right) f_{n\mathbf{k}\alpha}f^\star_{n'\mathbf{k}'\alpha'} \\ &+ \frac{J}{2N}\,T\sum_{\alpha''n''\beta''\mathbf{q}\;\omega_s}\left(\mathbf{S}_{\beta\beta''}\cdot\boldsymbol{\sigma}_{\alpha\alpha''}\right) f_{n\mathbf{k}\alpha}f^\star_{n''\mathbf{q}\alpha''}G_{n''\alpha''}\left(\imath\omega_s,\mathbf{q}\right)F_{\beta''}\left(-\imath\omega_s+\imath\omega\right)\Gamma^{\alpha''\beta''n''}_{\alpha'\beta'n'}\left(\mathbf{q},\mathbf{k}'\right),\end{aligned} \tag{9}$$

where G and F are the band fermion and the pseudofermion propagators respectively. The contribution of particle-hole channel is obtained by changing the sign of the frequency in one of the fermion propagators.

We find the solution for the vertex in the factorized form $\Gamma^{\alpha\beta n}_{\alpha'\beta'n'}(\mathbf{k},\mathbf{k}')=\Gamma_{\alpha\alpha';\beta\beta'}f_{n\mathbf{k}\alpha}f^\star_{n'\mathbf{k}'\alpha'}$. The spin matrix $\Gamma_{\alpha\alpha';\beta\beta'}$ is separated into distinct symmetry channels which couple the impurity moment to the fermions. From Eq. (9) we find

$$\begin{aligned}\Gamma^T_{\alpha\alpha';\beta\beta'} &= \Gamma^T_0\left(\delta_{\alpha\alpha'}S^0_{\beta\beta'}\right)+\Gamma^T_1\left(\boldsymbol{\sigma}_{\alpha\alpha'}\cdot\mathbf{S}_{\beta\beta'}\right)+\left(\Gamma^T_2+\Gamma^T_3\right)\sigma^0_{\alpha\alpha'}S^z_{\beta\beta'}-\left(\Gamma^T_2-\Gamma^T_3\right)\sigma^z_{\alpha\alpha'}S^0_{\beta\beta'} \\ &+\imath\Gamma^T_4\left(\sigma^x_{\alpha\alpha'}S^y_{\beta\beta'}-\sigma^y_{\alpha\alpha'}S^x_{\beta\beta'}\right)+\Gamma^T_5\left(\sigma^z_{\alpha\alpha'}S^z_{\beta\beta'}\right),\end{aligned} \tag{10}$$

where the label T refers to the sum of the particle-hole and particle-particle channels. In the equation above, the vertices Γ_1 and Γ_5 conserve the total spin, $\boldsymbol{S}+\boldsymbol{\sigma}$, of the impurity-conduction electron system, while the vertices Γ_2, Γ_3, and Γ_4 do not. This spin non-conservation is the main reason for the nontrivial results found below.

B. Impurity location.

The structure of the vertex depends on the location of the impurity. Consider, for example, a system with a square lattice, and the AFM ordering wave vector $\mathbf{Q}=(\pi,\pi)$. If the impurity is located at the point where the magnetization vanishes, midway between two nearest neighbors ($\mathbf{R}_i=(1/2,0)$ or $(0,1/2)$), $\exp\left(\mathbf{Q}\cdot\mathbf{r}_I\right)=\imath$. Then $f^*_{\mathbf{k}n\alpha}f_{\mathbf{k}n\alpha}=1$ and no change in Kondo screening occurs on going from the paramagnetic to the AFM state. This special behavior takes place only if the impurity is located at the point where the magnetization vanishes. For a general position of impurity $f^*_{n\mathbf{k}\alpha}f^\star_{n\mathbf{k}\alpha}\neq 1$, so that finite spin non-conserving vertices exist. In the following, we consider a substitutional impurity, $\mathbf{R}=0$.

C. One-loop Renormalization Group Analysis

We analyze the equations for the vertices at the one loop level, replacing the full propagators in Eq.(9) by their bare counterparts, G^0 and F^0. First note the spin-dependent elastic contribution to the pseudo-fermion self energy, shown in Fig. 1(c) $\Sigma_f(\sigma)\sim\sigma\rho J_z m\sinh^{-1}(-D/\gamma m)$, where ρ is the density of states (DOS), D is the bandwidth, and we assumed a constant DOS, N_0, in the band. Since we assume the Fermi surface is not nested, opening of the gap at parts of the FS close to the magnetic Brillouin Zone boundary leads to a build up of density of states, $D_\pm(\epsilon)$ for the '+' and '−' bands respectively, at the gap edge $E_\pm(\mathbf{k})\sim\gamma\,|m|$. The detailed shape of the DOS depends on the underlying band struc-

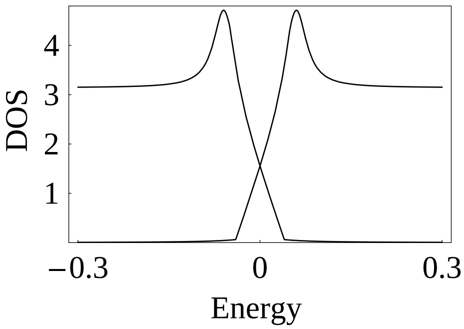

FIG. 2: Density of states for the two bands. For all numerical calculations, except when noted otherwise, the bandwidth is taken to be 10 and $\gamma m = 0.05$.

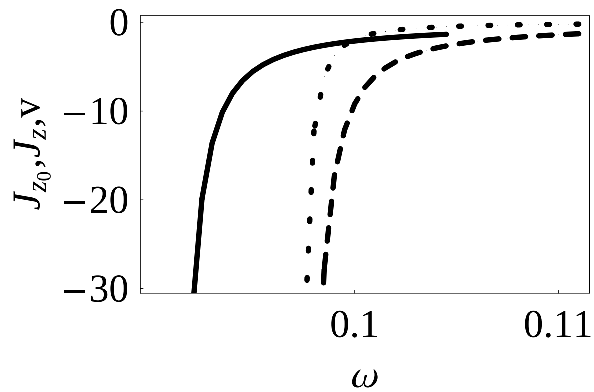

FIG. 3: Flow of $v(\cdot\cdot)$ and $J_z(---)$ where the initial values are $J_z = -0.4$ and $J_\perp = -0.4$. For comparison we also show the flow of $J_{z_0}(-)$in the absence of AFM order.

ture of the metal. Here, for simplicity and without loss of generality, we model $D_\pm(\epsilon) = D_1(\epsilon) + D_{2\pm}(\epsilon)$, where $D_1(\epsilon) = N_0 \mathrm{min}(|\epsilon|/\gamma m, 1)$ is the linearly suppressed DOS below the AF gap edge, and the Lorentzian contribution, $D_{2\pm}(\epsilon) = (a\gamma m/\pi)\left[(\epsilon \mp \gamma m)^2 + (\gamma m)^2\right]^{-1}$. For weak AFM, $\gamma m \ll D$, the choice $a = \gamma m N_0/2$ conserves the number of states. The resulting DOS for the particle-hole symmetric case, $D_-(-\epsilon) = D_+(\epsilon)$, is shown in Fig. 2: most of the lower(upper) band is occupied(empty). Despite this complex behavior of the density of states, evaluating $\Sigma_f(\sigma)$ with constant DOS is qualitatively accurate since there is no (logarithmic) frequency dependence to the self energy at this order. We use the full model density of states in computing the renormalization group flow and carrying out the variational ansatz below.

To one loop we find that $\Gamma_2^T = -\Gamma_3^T$, while to $O(J^2)$ $\Gamma_4^T = 0$. Both in the particle-hole and particle-particle channels the terms $\sigma^0 S^z$ and $\sigma^z S^0$ appear with opposite signs simply due to spin commutation rules. However, if the impurity is at a site with non-vanishing local magnetization, an additional relative sign change for the $\sigma^z S^0$ term between the two diagrams in Fig. 1 is due to the splitting of the band fermion spin states at the location of the impurity; hence the contributions of the two diagrams add in this channel, while canceling in the $\sigma^0 S^z$ channel. To this order in perturbation theory, the spin dependent self energy of the pseudofermions is zero, and hence $\Gamma_2^T = -\Gamma_3^T$; this is not true at higher orders. The particle-particle and particle-hole contributions to Γ_4 cancel to all orders due to particle-hole symmetry in this channel (recall that the magnetization m is chosen along z). In the absence of particle-hole symmetry, however, this spin non-conserving term is a relevant perturbation about the ordinary Kondo effect. With particle-hole symmetry, Γ_2^T and Γ_3^T are the only such relevant perturbations, while the asymmetry introduced through Γ_5^T is only marginal at the fixed point.

D. Renormalization Group (RG) Flow.

We now consider the renormalization of the coupling constants by integrating out the fermion states near the band edge. As explained above, the spin non-conserving $\sigma^z S^0$ interaction channel appears in the vertex. To investigate its flow, we introduce an effective exchange field acting only on the fermions: even though such an interaction is absent from the starting Hamiltonian, it is generated at one loop level and determines the RG flow by polarizing the conduction band at the impurity location. To this end we add to the Hamiltonian the term

$$H_V = -\frac{v}{2N}\sum_{\mathbf{k},\mathbf{k}',n,n'} S^0 \sigma^z_{\alpha\beta} f_{n\mathbf{k}\alpha} f^\star_{n'\mathbf{k}'\beta} a^\dagger_{n\mathbf{k}\alpha} a_{n'\mathbf{k}'\beta}\,. \quad (11)$$

In solving the flow equation we impose the initial condition that $v = 0$ and follow its evolution. Defining $h(\omega) = \gamma m/\sqrt{\omega^2 + \gamma^2 m^2}$, we find the RG equations for the coupling constants to order $O(J^2, v^2, Jv)$

$$\frac{\delta J_z}{2N} = -\left(f(\omega)\frac{J_\perp^2}{(2N)^2} - g(\omega)\frac{vJ_z}{(2N)^2}h(\omega)\right)\frac{\delta\omega}{\omega}\,, \quad (12)$$

$$\frac{\delta J_\perp}{2N} = -f(\omega)\frac{J_z J_\perp}{(2N)^2}\frac{\delta\omega}{\omega} + g(\omega)\frac{(v)J_\perp}{2(2N)^2}\frac{h(\omega)\,\delta\omega}{\omega}\,, \quad (13)$$

$$\frac{\delta v}{(2N)} = g(\omega)\left(\frac{v^2}{(2N)^2} + \frac{y}{(2N)^2}\right)\frac{h(\omega)\,\delta\omega}{\omega}\,, \quad (14)$$

where,

$$\begin{aligned} f(\omega) &= (D_+(\omega) + D_-(-\omega) + D_+(-\omega) + D_-(\omega))\,, \\ g(\omega) &= (D_+(\omega) + D_-(-\omega) - D_+(-\omega) - D_-(\omega))\,, \end{aligned}$$

and $y = \frac{J_z^2}{2} - J_\perp^2$. Note that for a paramagnetic metal with particle-hole symmetry $g(\omega) = 0$, and the equations reduce to those for the usual Kondo effect[1].

The flow of the exchange field v and the coupling constant J_z is shown in Fig. 3 for the density of states from Fig. 2. For comparison we also show the flow of J_{z_0} in

the absence of antiferromagnetic order. Note that both the Kondo coupling J, and the vertex v grow, and, at the one-loop level (with no self energy corrections), flow to strong coupling. This indicates that the Kondo screening is modified in the AFM state. To understand the nature of the fixed point we perform a calculation using a variational wavefunction motivated by the one loop results.

IV. VARIATIONAL ANSATZ.

To estimate the moment, binding energy and the impurity density of states in the ground state, we diagonalize the Hamiltonian within a restricted subspace spanned by the states ($\Downarrow$ and $\Uparrow$ are the states of the impurity spin, and $n = \pm$ as before)

$$\psi_{1n\mathbf{k}} = \frac{1}{\sqrt{2}}\left[\left(u_{\mathbf{k}} - nv_{\mathbf{k}}\right) a^{\dagger}_{n\mathbf{k}\uparrow} \otimes \Downarrow - \left(u_{\mathbf{k}} + nv_{\mathbf{k}}\right) a^{\dagger}_{\mathbf{k}\downarrow} \otimes \Uparrow\right],$$
$$\psi_{2n\mathbf{k}} = \frac{1}{\sqrt{2}}\left[\left(u_{\mathbf{k}} + nv_{\mathbf{k}}\right) a^{\dagger}_{n\mathbf{k}\uparrow} \otimes \Downarrow + \left(u_{\mathbf{k}} - nv_{\mathbf{k}}\right) a^{\dagger}_{n\mathbf{k}\downarrow} \otimes \Uparrow\right].$$

The states chosen here generalize those used to describe the ground state in the standard Kondo problem[12], which yield the same result for the ground state as the large N approximation[13] or slave Boson method[14]. In particular, the state ψ_1 for $u_{\mathbf{k}} = 1, v_{\mathbf{k}} = 0$ reduces to the singlet formed between the conduction electron and the impurity spin, while ψ_2 in the same limit becomes the triplet component. In contrast to the paramagnetic metal, here these two states are coupled by the exchange interaction, and hence both need to be considered when constructing the variational wave function.

We approximate $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ for all momentum states with the same energy, ϵ, by u_ϵ and v_ϵ, and work in basis states labeled by energy. Diagonalization within this subspace gives the eigenstates in the form: $\psi = \sum_{\tau\epsilon}\left(a\left(\epsilon,\tau\right)\psi_{1\tau\epsilon} + b\left(\epsilon,\tau\right)\psi_{2\tau\epsilon}\right)$. We use the density of states of the band fermions, Fig. 2, to numerically evaluate the energy and the variational coefficients a and b of the eigenstate with the lowest energy. In Fig. 4, we plot this energy for different values of the parameter γm and bare isotropic exchange coupling, J.

As expected, the binding energy decreases with increasing magnetic order m. We also estimate the total moment of the collective state by using the fermion spin operator, $\mathbf{s} = (1/2)\sum_{\mathbf{k},n} a^{\dagger}_{n\mathbf{k}\alpha}\boldsymbol{\sigma}_{\alpha\beta}a_{n\mathbf{k}\beta}$, and plotting the net moment $(\mathbf{S}+\mathbf{s})^2$ as a function of m in Fig. 4. Here $\mathbf{S}$ is the impurity spin operator, and the unscreened case corresponds to $\mathbf{S}^2 = 3/4$. As the antiferromagnetic order increases, the screening is less effective and the moment at the impurity site increases. Note significant change from the full screening in the absence of AFM order, $(\boldsymbol{S}+\boldsymbol{\sigma})^2 = 0$ when $m = 0$, to a substantial unscreened moment at $\gamma m = 0.01$. This results from the extreme sensitivity of Kondo screening to the low energy features of the conduction band.

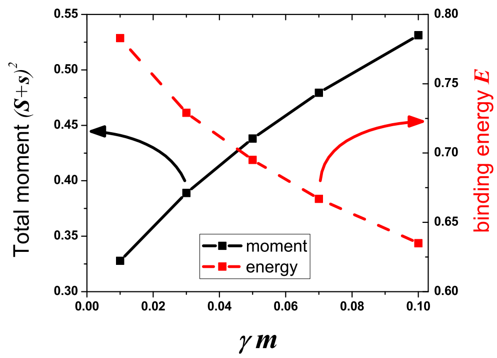

FIG. 4: Binding energy normalized to that in the absence of magnetic order, $E_0(\gamma m = 0)$ and net moment of the collective state for fixed value of the exchange coupling, $J = -0.04$.

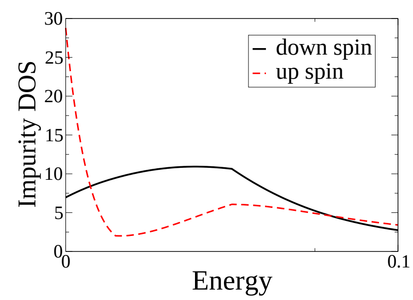

FIG. 5: Local spin-resolved DOS for the impurity located at the "up-spin" site for spins parallel(up) and antiparallel(down) to m where $\gamma m = 0.05$ and $J = -0.04$.

V. DENSITY OF STATES.

To estimate the single particle density of states we compute $n(\epsilon,\sigma) = \left\langle \sum_n a^{\dagger}_{\epsilon n\sigma}a_{\epsilon n\sigma}\right\rangle_{gs}$. The plot of the occupation for the two spins is shown in Fig. 5. Since the impurity sits at a site with the full symmetry of the square lattice, m defines the magnitude and direction of the electronic moment at the site in the absence of the impurity. Fig. 5 shows that the collective state formed by the impurity and the fermions leads to a splitting of the impurity density of states. The spin state antiparallel to m hybridizes with the fermions to give a rather broad peak shifted away from the chemical potential, while for the spins parallel to the sublattice magnetization, the density of states shows two peaks, one at the chemical potential while the other at the antiferromagnetic energy scale m. We expect that the spin-resolved local density of states in the antiferromagnetic state shows the same salient features even if computed fully self-consistently.

Our calculations have been performed in the magnetically ordered phase. We ignored the spin wave contribution, which becomes important near the magnetic phase transition; the effect of critical fluctuations leads to a multichannel Kondo problem near the critical point[15]. Coupling to the spin waves introduces a term of order $J^2 g\chi$ to one loop where g is the coupling

of order γm and χ the spin susceptibility of the form $1/(\omega^2+|\mathbf{q}-\mathbf{Q}|^2+\xi^{-2})$. Since in the ordered phase ξ is finite for the modes that couple to the fermions in the long-wavelength limit, the contributions due to spin waves are higher order in perturbation theory ($O(\gamma m J^2 \xi^2)$), and can be safely ignored here.

VI. SUMMARY.

To summarize we find that in an itinerant antiferromagnet, the Kondo screening of the impurity moment competes with a spin non-conserving coupling, which originates from the spin structure of the quasiparticles eigenstates in the AFM phase, and the nature of which depends on the local symmetry of the impurity site. Our result implies that in the heavy fermion AFM state the Kondo screening is incomplete; this is in contrast to a very recent variational Monte Carlo calculation for the Kondo lattice that found screening of the moment across the transition from paramegnet to antiferromagnet[10]. We have calculated by a simple variational method the residual ground state moment and its distribution as a function of energy which mimics what occurs in the antiferromagnetic heavy fermion state. This is the first step in understanding the ordered phase of Lattice Kondo model and its approach to criticality.

VII. ACKNOWLEDGEMENTS.

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